

Morpholine
110-91-8 | DTXSID2025688

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -1.82 °C

Global applicability domain: Inside

Local applicability domain index: 4.60e-01

Confidence level: 3.24e-01

Nearest Neighbors from the Training Set

Image not found

Morpholine

Measured: -4.90

Predicted: -1.82

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2,6-Dimethyl morpholine

Measured: -88.0

Predicted: -62.1

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4-Piperidinol, 1-methyl-

Measured: 29.0

Predicted: 41.0

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Bis(2-chloroethyl)amine
hydrochloride

Measured: 213

Predicted: 169

Image not found

Pyridine, 1,2,3,6-tetrahydro-

Measured: -48.0

Predicted: -35.6